

基本信息

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学术兼职	担任 ACS Nano, J. Mater. Chem. A, Chem. Asian J., ACS Applied Polymer Materials 等期刊审稿人	

教育背景

2010.09-2014.07	清华大学，化学专业，理学博士
2007.09-2010.07	湘潭大学，化学专业，理学硕士

工作经历

2018.04-至今	北京理工大学化学与化工学院，副研究员
2014.09-2018.02	香港科技大学，化学系，博士后

研究方向

1.	超分子组装和解组装机制的多尺度理论研究
2.	聚集诱导发光材料发光机理的理论预测及实验验证
3.	光催化水分解材料的结构与性能关系的理论研究
4.	有机半导体材料形貌与电荷传输性能关系的理论预测及实验验证

荣誉奖励

1	清华大学优秀博士学位论文
2	清华大学杜邦奖学金
3	湖南省优秀硕士学位论文
4	湘潭大学第十五届校长奖特等奖
5	湖南省优秀毕业生，湘潭大学优秀毕业生

承担项目

1.	国家自然科学基金青年项目，26 万，主持，2019/01-2021/12
2.	北京理工大学青年教师学术启动计划项目，40 万，主持，2018/04-2021/04

研究成果

主持国家自然科学基金项目 1 项；参与国家自然科学基金项目等 1 项。迄今在国内外学术刊物及会议上发表学术论文 53 篇，其中 SCI 收录 53 篇。

1.	将多尺度模拟方法与动力学网络模型相结合，模拟两亲性分子组装体形成机理，揭示逐步增长型和跳跃型两种组装路径通道，提出路径通道选择性决定的两亲性分子组装体形成机制
2.	将多尺度模拟方法与激发态衰减速率理论相结合，揭示分子组装体环境抑制分子内低频振动模式的电声子耦合，阻塞激发态的无辐射衰减通道来提高荧光效率的 AIE 机理，并提出通过电荷调节设计 AIE 荧光探针以选择性识别细胞膜和线粒体的策略，被实验所验证。
3.	采用多尺度模拟方法，研究不同形式外力作用下分子组装体堆积结构、转移积分及载流子迁移率的关系，提出将剪切力与正应力相结合调控分子堆积以设计高空穴迁移率低各向异性材料的新策略
4.	采用第一性原理方法，模拟光催化水分解材料的结构与性能关系

代表性论文

1.	F. F. Ma, X. Y. Zheng* , J. Xie, Z. S. Li.* Binding Properties of Cucurbit[7]uril to Neutral and Protonated Amino Acids: A Theoretical Study. <i>Int J Quantum Chem.</i> 2020, Accepted.
2.	X. Y. Zheng* , X. Z. Zeng, Z. W. Li. Multiscale simulation and kinetic network model analysis of the self-assembly of amphiphilic systems. <i>中国科学: 化学.</i> 2020, 50(9), 1118-1131. 【庆祝北京理工大学建校八十周年专辑】
3.	B. C. Lu, X. Y. Zheng* , Z. S. Li*. A Promising Photocatalyst of Water Splitting Reaction with Stable Sandwiched P ₄ O ₂ /Black Phosphorus Heterostructure and High Solar-to-Hydrogen Efficiency. <i>Nanoscale</i> 2020, 12, 6617-6623.
4.	X. Y. Zheng* , D. Wang*, W. H. Xu, S. Q. Cao, Q. Peng*, B. Z. Tang*. Charge Control of Fluorescent Probes to Selectively Target Cell Membrane or Mitochondria: Theoretical Prediction and Experimental Validation. <i>Mater. Horiz.</i> 2019, 6, 2016-2023 (selected as Back Cover and Highlighted by: Polymer-science)
5.	Z. Zhao [#] , X. Y. Zheng[#] (co-first author) , L. L. Du ¹ , Y. Xiong, W. He, X. X. Gao, C. L. Li, Y. J. Liu, B. Xu, J. Zhang, F. Y. Song, Y. Yu, X. Q. Zhao, Y. J. Cai, X. W. He, R. T. K. Kwok, J. W. Y. Lam, X. H. Huang, D. Phillips*, H. Wang* and B. Z. Tang*. Non-aromatic annulene-based aggregation-induced emission system via

	aromaticity reversal process. <i>Nat. Commun.</i> 2019, 10, 2952
6.	N. Zhao,* W. W. Gao, M. Zhang, J. F. Yang, X. Y. Zheng* , Y. Li, R. R. Cui, W. Yin, N. Li. Regulation of Circular Dichroism Behavior and Construction of Tunable Solid-State Circularly Polarized Luminescence Based on BINOL Derivatives. <i>Mater. Chem. Front.</i> 2019, 3(8), 1613-1618.
7.	D. Wang,* M. M. S. Lee, W. H. Xu, G. G. Shan, X. Y. Zheng* , R. T. K. Kwok, J. W. Y. Lam, X. L. Hu,* B. Z. Tang.* Boosting Non-Radiative Decay to Do Useful Work: Development of Multi-Modality Theranostic System from AIEgen. <i>Angew. Chem. Int. Ed.</i> 2019, 58 (17), 5628-5632.
8.	B. C. Lu, X. Y. Zheng* and Z. S. Li*. Few-layer P ₄ O ₂ : A Promising Photocatalyst for Water Splitting. <i>ACS Appl. Mater. Interfaces.</i> 2019, 11(10), 10163–10170
9.	Y. X. Lei, W. B. Dai, Z. Q. Liu, S. Guo, Z. X. Cai*, J. B. Shi, X. Y. Zheng* , J. G. Zhi, B. Tong, Y. P. Dong*. A Novel Strategy for Realizing Dual State Fluorescence and Low-Temperature Phosphorescence. <i>Mater. Chem. Front.</i> 2019, 3(2), 284-291.
10.	H. K. Zhang [#] , X. Y. Zheng[#] (co-first author) , R. T. K. Kwok, J. Wang, N. L. C. Leung, L. Shi, J. Z. Sun, Z. Y. Tang, J. W. Y. Lam, A. J. Qin*, B. Z. Tang*. In situ monitoring of molecular aggregation using circular dichroism. <i>Nat. Commun.</i> 2018, 9(1), 4961
11.	X. Y. Zheng , L. Z. Zhu, X. Z. Zeng, L. M. Meng, L. Zhang, D. Wang, X. H. Huang*. Kinetics-Controlled Amphiphile Self-Assembly Processes. <i>J. Phys. Chem. Lett.</i> 2017, 8, 1798-1803
12.	H. K. Zhang, X. Y. Zheng , N. Xie, Z. K. He, J. K. Liu, N. L. C. Leung, Y. L. Niu, X. H. Huang, K. S. Wong, R. T. K. Kwok, H. H. Y. Sung, I. D. Williams, A. J. Qin, J. W. Y. Lam, B. Z. Tang*. Why Do Simple Molecules with “Isolated” Phenyl Rings Emit Visible Light? <i>J. Am. Chem. Soc.</i> 2017, 139, 16264-16272 (Highlight by Nature Reviews Chemistry)
13.	H. Q. Peng, X. Y. Zheng , T. Han, R. T. K. Kwok, J. W. Y. Lam, X. H. Huang, B. Z. Tang*. Dramatic Differences in Aggregation-Induced Emission and Supra-molecular Polymerizability of Tetraphenylethene-Based Stereoisomers. <i>J. Am. Chem. Soc.</i> 2017, 139, 10150-10156
14.	X. Y. Zheng , Q. Peng*, L. Z. Zhu, Y. J. Xie, X. H. Huang*, Z. G. Shuai*. Unraveling the Aggregation Effect on Amorphous Phase AIE Luminogens: A Computational Study. <i>Nanoscale</i> 2016, 8, 15173-15180 (Inside Front Cover)
15.	X. Y. Zheng , H. Geng, Y. P. Yi, Q. K. Li, Y. Q. Jiang, D. Wang*, Z. G. Shuai*. Understanding Lattice Strain-Controlled Charge Transport in Organic Semi-conductors: A Computational Study. <i>Adv. Funct. Mater.</i> 2014, 24, 5531-5540
16.	S. Feng [#] , X. Y. Zheng[#] (co-first author) , D. Wang, Y. Y. Gong, Q. T. Wang, H. T. Deng*. Systematic Analysis of Reactivities and Fragmentation of Glutathione and Its Isomer GluCysGly. <i>J. Phys. Chem. A</i> 2014, 118, 8222-8228
17.	X. Y. Zheng , D. Wang*, Z. G. Shuai*. Coarse-grained Molecular Dynamics Simulations of Photoswitchable Assembly and Disassembly. <i>Nanoscale</i> 2013, 5, 3681-3689

18.	X. Y. Zheng , Z. G. Shuai*, D. Wang*. Anion-Binding Properties of π -Electron Deficient Cavities in Bis(tetraoxacalix[2]arene[2]triazine): A Theoretical Study. <i>J. Phys. Chem. A</i> 2013, 117, 3844-385.
19.	K. Liu [#] , X. Y. Zheng [#] (co-first author), A. Z. Samuel, S. G. Ramkumar, S. Ghosh, X. X. Tan, D. Wang, Z. G. Shuai, S. Ramakrishnan, D. S. Liu, X. Zhang*. Stretching Single Polymer Chains of Donor-Acceptor Foldamers: Towards the Quantitative Study on the Extent of Folding. <i>Langmuir</i> 2013, 29, 14438-14443
20.	X. Y. Zheng , D. Wang*, Z. G. Shuai, X. Zhang. Molecular Dynamics Simulations of the Supramolecular Assembly between an Azobenzene-Containing Surfactant and α -Cyclodextrin: Role of Photoisomerization. <i>J. Phys. Chem. B</i> 2012, 116, 823-832
21.	X. Y. Zheng , X. Y. Wang*, K. Q. Shen, N. Q. Wang, Y. M. Peng. Molecular Design of a "Molecular Syringe" Mimic for Metal Cations using a 1,3-alternate Calix[4]arene Cavity. <i>J. Comput. Chem.</i> 2010, 31, 2143-2156
22.	X. Y. Zheng , X. Y. Wang*, S. F. Yi, N. Q. Wang, Y. M. Peng. Density Functional Theory Study of 1,3-alternate-25,27-bis(1-methoxyethyl)-calix[4]arene-N-azacrown-5 and Their Complexes with Alkali Metal Cations: Na ⁺ , K ⁺ , Rb ⁺ . <i>J. Comput. Chem.</i> 2010, 31, 1458-1468
23.	X. Y. Zheng , X. Y. Wang*, S. F. Yi, N. Q. Wang, Y. M. Peng. Density Functional Theory Study of the Free and Tetraprotonated Spheroidal Macrotricyclic Ligands and the Complexes with Halide Anions: F ⁻ , Cl ⁻ , Br ⁻ . <i>J. Comput. Chem.</i> 2010, 31, 871-881
24.	X. Y. Zheng , X. Y. Wang*, S. F. Yi, N. Q. Wang, Y. M. Peng. DFT Study of the Carbon- and Nitrogen-Pivot Lariat Crown Ethers and Their Complexes with Alkali Metal Cations: Na ⁺ , K ⁺ . <i>J. Comput. Chem.</i> 2009, 30, 2674-2683